# 2-Methylphenanthrene

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|---------------|-------------|
| 2531-84-2   D | TXSID102564 |
|               |             |

### **Model Performance**

| Model | Data |
|-------|------|

# Weighted KNN model

| 5-fold CV (75 | 5%)  | Training (75%) |      | Test (25%) |      |  |
|---------------|------|----------------|------|------------|------|--|
| Q2            | RMSE | R2             | RMSE | R2         | RMSE |  |
| 0.85          | 0.69 | 0.86           | 0.67 | 0.86       | 0.78 |  |

#### **Model Results**

Predicted value: 4.11

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 7.21e-01

## Nearest Neighbors from the Training Set

Image not found
2-Chlorobiphenyl
Measured: 4.53
Predicted: 4.26

Image not found Fluorene

Measured: 4.18 Predicted: 2.77

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Benzene, 1-chloro-3-phenoxy-

Measured: 4.75 Predicted: 3.14